

1,3-diphenyl-1,3-diazetidine  
74949-76-1 | DTXSID60321268

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

## Model Results

**Predicted value:**  $4.83\text{e-}11$  cm<sup>3</sup>/molecule\*sec

**Global applicability domain:** Outside

**Local applicability domain index:**  $1.28\text{e-}01$

**Confidence level:**  $6.97\text{e-}01$

## Nearest Neighbors from the Training Set

Image not found

1,4-Benzoquinone

**Measured:**  $4.60\text{e-}12$

**Predicted:**  $5.97\text{e-}12$

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1,3,5-Cycloheptatriene

**Measured:**  $9.69\text{e-}11$

**Predicted:**  $1.00\text{e-}10$